IN SILICO ENZYME ENGINEERING – THE IMPORTANCE OF FAST AND ACCURATE ALGORITHMS

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Computer simulations are already widely used to rationally engineer new enzymes with improved properties. But if we can accurately screen millions of enzyme variants in a computer, then we can move into a new generation of *in silico* enzyme evolution. At ZYMVOL we are to be able to produce, model and rank protein-substrate interactions (including full protein dynamics) for over 50.000 enzyme variants per day. We have accelerated physics-based simulations, and combined experimental data with quantum approaches to develop a highly predictive computational platform. Our ZYMEVOLVER software can effectively reduce experimental validation to a few hundred variants and enzyme optimization campaigns to less than 6 months.

We will illustrate how we are creating custom-made enzymes for industrial applications.